

## LabKey for Multicenter R&D on Biofuels and Bio-based Products

Jim Collett LabKey User Conference 2019



![](_page_0_Picture_4.jpeg)

PNNL is operated by Battelle for the U.S. Department of Energy

PNNL-SA-148026

EN	Ξ	RGY	.GOV		
Office	of	Energy	Efficiency &	Renewable	Energy

**Bioenergy Technologies Office** 

### POET-DSM Project Liberty Cellulosic ethanol from corn stover

![](_page_1_Picture_3.jpeg)

The DOE's Bioenergy Technologies Office supports R&D on the production of biofuels from a variety of feedstocks.

![](_page_1_Picture_5.jpeg)

LanzaTech, PNNL, & Partners Steel mill flue gas, biomass to jet fuel

![](_page_1_Picture_7.jpeg)

PNNL & Partners Sewage sludge, manure, and algae to renewable diesel

![](_page_1_Picture_9.jpeg)

![](_page_1_Picture_10.jpeg)

![](_page_1_Picture_11.jpeg)

![](_page_1_Picture_12.jpeg)

![](_page_1_Picture_13.jpeg)

![](_page_2_Picture_0.jpeg)

The Feedstock-Conversion Interface Consortium (FCIC) seeks to understand and mitigate biomass variability and its effects on biorefinery performance.

![](_page_2_Picture_2.jpeg)

![](_page_2_Figure_3.jpeg)

The FCIC has recently begun using LabKey Professional Plus Edition running on AWS Linux to integrate experimental data from 8 national laboratories.

![](_page_3_Picture_1.jpeg)

![](_page_3_Picture_2.jpeg)

### 1 - FCIC 🗸

- E FCIC Task Work
  - FY18 FCIC Task Work
  - T.01.00 Materials of Construction
  - T.02.00 Feedstock Variability
  - T.03.00 Materials Handling
  - T.04.00 Data Integration & Quality by Design
  - T.05.00 Feedstock Preprocessing
  - T.06.00 Direct Biomass Liquefaction
  - T.07.00 Low-Temperature Conversion
    - T.08.00 Cross-Cutting Analysis

![](_page_3_Figure_14.jpeg)

LabKey Server is also running within the firewalls of PNNL, INL, NREL, ORNL, and LBNL to stage data for uploading to the FCIC LabKey Data Hub, or to manage other DOE project data.

![](_page_4_Picture_0.jpeg)

## **CIC** Task 1. Materials of Construction

### Subtasks

- **1.1. Equipment Wear in Preprocessing**
- **1.2. Equipment Wear in Low-Temperature Pre-conversion**
- **1.3 Mechanics of Wear**
- **1.4 Materials Mitigation of Deposit-lead** Feeder Plugging in HT Pre-conversion

Jun Qu, Kyungjun Lee, and Jim Keiser (ORNL)

	Subtask Objectives: Using a systematic quality-by-desi preprocessing equipment, such as hammer and knife r	gn approa nills, and s	ch with integrate hare with the bio	d efforts of cl mass industr	naracter /.	rization, mo	odeling, a	nd testing	to funda	mentally	understa	and an		
	Technical Approach:	Assay List / EDS_SEM_Image_Analysis Batches / EDS_SEM_Image_Analysis Runs												
	<ul> <li>Characterize extrinsic ash and intrinsic compound</li> </ul>	EDS_	SEM_Imag	ge_Analy	sis R	esults	C T.01.0	1 EQUIP	MENT W	EAR IN F	PREPROC	ESSING		
	<ul> <li>Investigate the wear mechanisms of the steel has</li> </ul>	MANAGE A		IEW BATCHES	VIEW	RUNS ⊫ V	IEW RESULT	S VIEW	COPY-TO-	STUDY HI	STORY »	VIEW EXC		
	<ul> <li>Develop mitigation strategies by biomass modified</li> </ul>	m	- 14 - 2	- Copy Te	Study	Import Da	ata Rep	laced Filter	- B					
	<ul> <li>Evaluate candidate mitigations by bench tribo-te</li> </ul>		ale Sample ID	Image File	wt% C	wt% Fe	wt% Mg	wt% Na	wt% N	wt% O	wt% Si	wt% Al	at?	
	<ul> <li>Demonstrate the feasibility of top mitigations on</li> </ul>	-	0 0		66.95	0	0.10	0.05	0.02	25.02	0 4 4 E	0.09	7	
			2 2_1		62.03	0.56	0.19	0.03	1.11	29.16	5.98	0.98	7	
			3 3 1		49.88	2.54	0.36	0.19	1.89	28.94	13.08	3.13	6	
	Assay List		3 3_2		55.55	1.93	0.22	0.14	1.85	28.19	10.43	1.68	6	
-			3 3_3		16.01	1.6	0.0	0.0	1.43	40.01	40.69	0.26	2	
	🎟 👻 🕨 💌 New Assay Design 🛛 Manage As		4 4_1	8 B	35.32	4.32	0.39	0.17	1.96	32.65	22.05	3.14	4	
	a - E - Hen Assay Sealgh - Mahage As		4 4_2		49.32	3.44	0.42	0.09	3.61	33.03	8.32	1.77	5	
	× T Name IS ONE OF (EDS_SEM_Image_An		4 4_3		28.56	1.91	0.47	0.11	0.86	20.79	42.1	5.19	4	
	Name 🕇 🌢 💿 Descri		4 4_4	222	35.65	1.78	0.27	0.04	1.82	32.9	26.82	0.72	4	
	EDS_SEM_Image_Analysis		4 4_5		32.3	1.93	0.3	0.04	2.25	34.57	27.79	0.83	4	
	Wear_Particle_Size_Fraction_Distribution		4 4_6		68.17	0.65	0.09	0.04	0.89	24.96	4.27	0.94	7	
	Wear Particle Volume Fraction Distribution		23 23_1		36.68	1.6	0.09	0.13	1.0	33.24	26.44	0.83	4	

![](_page_5_Picture_0.jpeg)

### Datasets

#### Assays

Ash (%, 750C) Ash Speciation (%oxide of ash basis) Compositional Analysis-NREL, NIR model

- 2.1. Variability, Transport and Synergistic Impacts of Inorganic Species
- 2.2 Quantify and Understand Variability of Molecular-scale Organic Attributes
- 2.3 Feedstock Variability at the Micro-scale
- 2.4 Feedstock Variability at the Macro-scale
- 2.5: Data Analytics for Identifying CMAs\* of Feedstocks
- \*Critical Material Attributes within the Quality by Design framework.

Amber Hoover (INL) and Erin Webb (ORNL)

Assays (Continued) Moisture (%, 105C) Moisture (%, 107C)

#### Assays (Continued)

Particle Size Distribution-Ro Tap Images

![](_page_5_Figure_14.jpeg)

The FCIC LabKey Data Hub uses INL's Bioenergy Feedstock Library (BFL) as a biomass specimen archive.

- BFL is a custom app on MS SQL Server
- Currently hyperlinking via GUIDs
- Plans call for automated sample registration

![](_page_6_Picture_4.jpeg)

![](_page_6_Picture_5.jpeg)

![](_page_7_Picture_0.jpeg)

## **fcic** Task 3. Materials Handling

- 3.1 Continuum Modeling for Feedstock-Handling
- 3.2 CFD modeling for reliable operation of screw feeders
- 3.3 Discrete Element Models for Fundamental Particle Flow Physics & Upscaling
- 3.4: Particle friction and cohesion measurement
- 3.5: Bulk Flow Characterization

![](_page_7_Picture_7.jpeg)

Jordan Klinger (INL) and Troy Semelsberger (LANL)

Bulk Flow Characterization Study Characterization

Data Views 🖋		
Filter name, category, etc.	E	Mine
Name	Details	Access
G Uncategorized		
I Surface Area vs. Chemical Composition	:=	public
La Surface Area vs. SO3 Chart	=	public
Les Surface Area vs. Fe2O3	=	public
I GUID_Match	=	
III NREL Compositional Analysis 2	=	
III Nitrogen_Surface_Area_3	=	
GUIDs SA Oxides	=	private
III GUIDs_N2SA_Fe203_K20_Mg0_S03	:=	public

Surface Area vs. Chemical Composition 🗅 Bulk Flow Characterization

⊞ <b>- ±</b> -	0					1 - 10	)0 of
GUIDs SA Oxides							
LANL GUID C	NREL GUID ©	Composition Sample ID ©	Average N2 Surface Area M2 G	FeSO3 wt% O	K20 wt% 📀	Mg O 🗢	S03
cfe01cb9-8d28-f34c- 8987-970c4aafc541	ad54c824-1ee6-5642- 8981-6aec8bdb566a	LMLA_Bale12_Segment3	0.667	1.61	13.22	4.4	ı
f2772330-12f2-bc40- a6d0-218d1051bb4e	dcbcc9a4-525d-294d- a85d-aa0c5a018536	LMLA_Bale11_Segment6	0.732	1.71	11.09	3.22	2
fa8f3731-0154-1b41- 8f89-b4b20808bc93	61f4e57e-ece4-5848- a0b4-10f86f7e698d	LMLA_Bale11_Segment4	0.746	1.99	8.94	3.27	,
6a11eb80-b893-d349- a1c4-d7e8043a439c	a76697e6-2979-0849- 8751-fba9c3d3420b	LMLA_Bale10_Segment4	0.752	1.73	11.72	3.87	,
1c2a8dcf-1ea4-a448- 8a9b-591589f2502d	4fa560ea-b90d-da4f- a5ab-077afca7d535	LMLA_Bale12_Segment4	0.772	1.77	12.93	3.71	I

![](_page_7_Figure_13.jpeg)

Surface Area vs. Fe2O3 C Bulk Flow Characterization

![](_page_8_Picture_0.jpeg)

- 5.1 Quality by Design for Low-Temperature Preprocessing Unit Operations
- 5.2 Quality by Design for High-Temperature Preprocessing Unit Operations
- 5.3 Preprocessed Feedstock Bulk Transport Phenomena Modeling
- 5.5 Machine Vision for Feedstock Quality Identification
- Vicki Thompson and Neal Yancey (INL)

#### CMA Identification for TCPDU Pyrolysis Performance FY19Q3 Results Summary 🖋

From the FY18 HT baseline runs, seven of the supersacks of loblolly pine chips and residues that were preprocessed at INL and then converted to pyrolysis oils at NREL were labeled for three conversion processes efficiency metrics: 'On Stream', a continuous variable representing the ratio of the time on stream divided by the time on stream plus the downtime; 'Char Removal', a categorical binary variable indicating whether a run needed to be stopped to clean out either cyclones or char bridging; and 'Feedtrain Bridging', a categorical binary variable indicating whether there were bridging problems in the feedtrain during sample processing. The properties of the raw materials were assessed as potential explanatory variables for these three efficiency metrics including: moisture, total ash, ash speciation, elemental C, H, N, O, and S, volatiles, and particle size distribution factors (D10, D50 and D90).

There was not an obvious visual correlation or pattern between any of these factors alone and the three efficiency metrics. When using a multivariate least squares linear regression approach the 'On Stream' metric could be linearly correlated to a combination of three factors: moisture, particle size factor of D50, and total carbon. All three of these factors contribute significantly (considering p

![](_page_8_Figure_9.jpeg)

Figure 1. Multivariate linear fit explaining 'On Stream' variability using moisture, particle size factor of D50, and total carbon.

For the 'Char' and 'Feedtrain' efficiency metrics, a Response Screening methodology was used to asses any strongly relating factors; however, as the data was limited, a good fit was not obtained for either metric. It is instructive to look at the factors (Table 1) that did contribute to those models (p

Table 1. Response screening results using a binary response for char (Yes: char formation resulted in shutdown or No: char formation did not result in shutdown) and Feedtrain (Yes, bridging occurred during a run causing shutdown or No: bridging did not occur to an extent requiring shutdown)

Char Response Factor	PValue	Feedtrain Response Factor	PValue
Titanium	0.002	Nitrogen	0.004
D90	0.03	Sodium	0.02
		Halogens	0.03

-Attached Files-

![](_page_9_Picture_0.jpeg)

## **fcic** Task 6. High-Temperature Conversion (Pyrolysis)

- 6.1 Biomass Thermal Transformations During High-Temperature Feeding
- 6.2: Impacts of Forest Residue Variability on Critical Pyrolysis Product Attributes
- 6.3 Mesoscale Simulation of High-Temperature Conversion
- 6.4 High-Temperature Reactor Scale Modeling
- Danny Carpenter (NREL) and Mike Thorson (PNNL)

![](_page_9_Figure_7.jpeg)

## **CIC** Task 7. Low-Temperature Conversion (Bioconversion)

7.1 Real-Time Monitoring of Deacetylation

- 7.2 Impacts of Feedstock Variability on Biological Sugar Conversion
- 7.3 Impacts of Feedstock Variability on Biological Lignin Conversion
- 7.4 Modeling Impacts of Feedstock Variability on Low-Temperature Pathways
- 7.5 DMR Materials Preparation
- 7.6 Chemical Lignin Conversion
- 7.7 Deacetylation Kinetic Model Development

Jeff Linger (NREL) and Deepti Tanjore (LBL)

Assay List
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Α.

Β.

C.

	Reports New Assay Design Manage Assays 🖨 1-6	of 6 📼
Name 📤 🛇	Description	Туре 🛇
Analytical	Analytical results catalogued by unique Sample ID.	Genera
Mass Spec	Mass spectrometer data. This is a general datastream, searchable by datetime and sample port ID.	Genera
Master Log	Master metadata and notebook records, including sample IDs, for each experimental run.	Genera
Media	Media component/recipe data. All unique recipes have unique IDs.	General
Process	Process data from MFCS	Genera

	. <b>.</b> .	Û	± - Co	ру То S	tudy In	nport Da	ta Re-import R	un Re	place	d Filter 👻	0								
×	Run = 177	User	Notes ©	OD	YSI	YSI	Sample ID	Sample	Run	Description	Start datetime	End datetime	Inoculation Time	Inoculation	Fermenter	Media	Starting	Strain	Mass
		Name	10100	(600 nm)	Glucose (g/L) ©	Xylose (g/L)	Campie is	Size (mL) ©	ID ©	O			0	Vol (mL)	ID ©	ID ©	Vol (L)	0	Spec Sample ID
	2018-10-16 13:00	I rspiller	inoculated	0.75			201810160017		3	40°C, 5.5 pH, 400 rpm	2018-10-16 13:00	2018-10-22 12:30	2018-10-16 13:00	10.6	1B1		0.3	YC-1	F3
	2018-10-16 16:00	I rspiller		1.33			201810160018		3	40°C, 5.5 pH, 400 rpm	2018-10-16 13:00	2018-10-22 12:30	2018-10-16 13:00	10.6	1B1		0.3	YC-1	F3
	2018-10-17 08:00	I rspiller		3.86			201810160019		3	40°C, 5.5 pH, 400 rpm	2018-10-16 13:00	2018-10-22 12:30	2018-10-16 13:00	10.6	1B1		0.3	YC-1	F3

Anal	Analytical Results DT.07.02												
Analytic	cal results catalo	ogued by unique Sar	mple ID.										
MANAGE	MANAGE ASSAY DESIGN > VIEW BATCHES > VIEW RUNS > VIEW RESULTS > VIEW COPY-TO-STUDY HISTORY >												
	· 🔟 ·	û 🛓 -	Copy To Study Import I	Data Replaced Filter 💌	Ð								
	Sample ID 🗢	Date 📀	Glucose (g/L) 📀	Acetoin (g/L) 💿	BDO (g/L) 💿	Glycerol (g/L)	Xylose (g/L) 💿	Meso BDO (g/L) 🗢	SS BDO (g/L) C				
	201810160001	2019-01-01 00:00	74.90938374951143	1.845626660642323	0.4733268108833657	0.1969545226547498	34.70718183981444	0.3996729920403159	0.0736538188430497				
	201810160002	2019-01-01 00:00	71.9094199336699	3.6201470885507656	0.6068808987387777	0.21878615481301347	34.61680096642983	0.5170411877663936	0.0898397109723841				
	201810160003	2019-01-01 00:00	0.3736847623704823	0.6781079731921322	41.22377716875911	3.6551089304785553	21.86218617922208	35.95062748263425	5.27314968612485				

# Considerations in using LabKey for multi-center, time-series process and sample data for industrial biomanufacturing R&D

- How best to define Subject/Participant across LK Studies at multiple scales?
- Aligning start datetimes of process data to place all unit operations and samples on same elapsed time basis
- Windowing functions e.g., over(), PARTITION BY not in LabKey SQL; must use R for timestamp matching
- What's the interest in clinical time series data in LK community? ICU, surgery data?

Clinical parallels - Biomass deconstruction is kind of like mammalian digestion

![](_page_11_Figure_6.jpeg)

![](_page_11_Picture_7.jpeg)

At PNNL, we are using LabKey to integrate Process Analytical Technology (PAT) data with sample and event data.

![](_page_12_Picture_1.jpeg)

![](_page_12_Picture_2.jpeg)

## **Bench to Pilot Scale Bioreactors**

A new low-cost, high-resolution Raman spectroscopy analyzer is being adapted for predicting bioreactor broth components (i.e., glucose) in real time.

Fed-batch control of the production of citric acid from corn stover hydrolysate by the oleaginous yeast *Yarrowia lipolytica* was recently achieved using this approach.

![](_page_13_Picture_2.jpeg)

![](_page_13_Figure_3.jpeg)

Hours After Inoculation

Bioreactor broth is recirculated through a Raman flow cell.

![](_page_14_Figure_1.jpeg)

Pacific Northwest Loading HPLC data into LabKey Assay no problem even if samples taken every 30 minutes – single spreadsheet, easy to handle

![](_page_15_Picture_1.jpeg)

![](_page_15_Picture_2.jpeg)

#### Assay List / HPLC\_Sugars\_OrgAcids\_BPD Batches / HPLC\_Sugars\_OrgAcids\_BPD Runs HPLC Sugars OrgAcids BPD Results C Automation Dev

E	EASSAY DESIGN 👂 VIEW E		Copy To Study	mport Data	Replaced Filter 👻		▶ VIEV	VEXCLU	DED DAT	A 🖻
<b>v</b> •	Sample ID 📀	Culture Age ©	Strain Line ID 💿	Experiment	Date 💿	Glucose (g/L) ©	Xylose (g/L)	Citric Acid (g/L)	Xylitol (g/L)	Fru (g/
	B500mL_003_ACF_002	1.76	Y- 7208_B500mL_003	B500mL_003	2019-09-06 16:49	27.54	15.59	0.06	0.43	
	B500mL_003_ACF_004	3.26	Y- 7208_B500mL_003	B500mL_003	2019-09-06 18:19	26.83	14.96	0.05	0.42	
•	B500mL_003_ACF_006	4.76	Y- 7208_B500mL_003	B500mL_003	2019-09-06 19:49	26.56	14.88	0.06	0.37	
	B500mL_003_ACF_008	6.26	Y- 7208_B500mL_003	B500mL_003	2019-09-06 21:19	26.33	14.96	0.06	0.38	

In a recent bioreactor run, the Raman analyzer generated a text file every 3 minutes = 480 files/day, 3360/week

Raw Counts Dark Subtracted

42396.3333 42214

41848.3333 41668

41462 41243.6667

41013 40803.3333

40509 40319.3333

39058.6667 38867

38355 38122.6667

37713.3333 37510

37374.6667 37173

36783.3333 36572

36698.3333 36276.6667

37986.3333 37780.3333

37102.6667

36898 36670

39752.3333 39552.3333

38846.3333 38573.3333

36883.3333

40158 39958

Software Version: 2.0.6.4 Unit SN: AIO-M73-0032 Spectrometer SN: 5346 Date: 3/20/2019 20:14:06 Data Line Index: 25 Spectral Points: 1939 Integration time (ms): 2000 Averages: 3 Delay (ms): 180000 Sequence Number: 1 dark subtract Processing: Laser Power (mW): 405 Laser Current (mA): 852 Laser Diode Temp (C):25 Laser Case Temp (C): 29.4 System Temp (C): 30.3 Spectrometer Temp (C): 27.6 CCD Temp (C): -0.008 Secondary Temp (C): 20.006 Heatsink Temp (C): 26.165 CCDPCB Temp (C): 38.997 SecondaryPCB Temp (C): 39.53

RamanShift

203.8746

206.1087

208.3423

210.5752

212.8077

215.0396

221.7321

223.9618

226.191

230.6477

232.8752

235.1022

237.3287

239.5546

241.7799

217.271

201.64 42888.6667 42703.6667

39364 39156.6667

Wavelength

798.0308

798.1732

798.3155

798.4579

798.6003

798.7427

798.8851

799.0275

799.3125

799.4549

799.5974

799.8825

800.1676

800.3102

800.4528

800.5954

800.025

799.17 219.5018

799.74 228.4196

![](_page_15_Picture_7.jpeg)

## 1939 wavenumbers & Intensities

Python script had to be used for parsing Raman data and writing into a Assay during uploading Each transformed spectral read is loaded into a LabKey Assay with 1939 intensities stored in a multiline text field. Wavenumbers rarely change, so they are stored separately in a List.

![](_page_16_Picture_1.jpeg)

				Assay	y List / F	Raman_Tra	insform	ation Bat	tches / F	Raman_T	ransforma	tion Runs									
				Rar	nan	Transf	orma	ation I	Result	S COL	utomatio	n Dev									
				nai	nan_	mansi	onne		Court		acomacio	1_000									
				Trans	formatio	n of a zip f	ile of ra	aw spectr	a to a Lal	oKey ass	ay with R	and Python									
				MANA	GE ASSAY	DESIGN )	VIEW B	BATCHES )	VIEW R	UNS )	VIEW RESUL	.TS VIEW (	COPY-TO-S	TUDY HIS		XCLUDED DA	TA 🕨				
•	Labilev				· ·	-	ŵ	± -	Сору То	Study	Import D	ata Replac	ed Filter					1-1	00 of 6.771 👻	<	>
Au	tomation_Dev 🗸				Tile N			0	Flamoad	Data		Internetien	A	Lanar	Maria and and	Out is at ID		Dresses	Ot ant Time a		Datah
issa lam	ay List / Raman_Transformation Batches / Ra an_Transformation Results 🗅 Automation_De	aman_Transf W	formation Runs		File Na	ame			Time	Date		Time	Of	Laser Power	vvavenumbers	Subject ID	)	ID O	Start Time	N N	Name
ran	sformation of a zip file of raw spectra to a La	bKey assay	with R and Python						(h) 🔍					© ○							0
Œ	🛛 - 🖄 - 📋 📥 - Copy To Study Impo	rt Data Re-	-Import Run Replaced Filter- Exclude		B30.3	5_2s3av40	0mw_0	0000.txt	5.30	2019-0	3-20 20:10	2000.00	3.00	400.00	2.0.6.4	B30_35_A	TCC32359_WT_1	B30_35	2019-03-20 14:	52 B	330.35
	default This grid view has been modified.	Revert Edit	Save		B30.3	5_2s3av40	0mw_0	0001.txt	5.35	2019-0	3-20 20:14	2000.00	3.00	405.00	2.0.6.4	B30_35_A	TCC32359_WT_1	B30_35	2019-03-20 14:	52 B	330.35
(×.	TRun = 204	Flansed Inte	neities		B30.3	5_2s3av40	0mw_0	0002.txt	5.41	2019-0	3-20 20:17	2000.00	3.00	405.00	2.0.6.4	B30_35_A	TCC32359_WT_1	B30_35	2019-03-20 14:	52 B	330.35
		Time (h) ©			B30.3	5_2s3av40	0mw_0	0003.txt	5.46	2019-0	3-20 20:20	2000.00	3.00	405.00	2.0.6.4	B30_35_A	TCC32359_WT_1	B30_35	2019-03-20 14:	52 E	330.35
		7, 7, 328	, 10, 9, 8, 8, 10, 10, 7, 9, 9, 12, 11, 13, 20, 18, 15, 26, 24 15, 32824, 32578, 32400, 32232, 32085, 32033, 318		B30.3	5_2s3av40	0mw_0	0004.txt	5.52	2019-0	3-20 20:23	2000.00	3.00	400.00	2.0.6.4	B30_35_A	TCC32359_WT_1	B30_35	2019-03-20 14:	52 B	330.35
		277 217 217	73, 27721, 27394, 27173, 27109, 26909, 26441, 261 82, 21799, 21730, 21804, 21760, 21759, 21697, 215 60, 21920, 22045, 22466, 22218, 22031, 21819, 217		B30.3	5_2s3av40	0mw_0	0005.txt	5.57	2019-0	3-20 20:27	2000.00	3.00	405.00	2.0.6.4	B30_35_A	TCC32359_WT_1	B30_35	2019-03-20 14:	52 E	330.35
		216 221	29, 21604, 21597, 21668, 21584, 21365, 21544, 215 11, 22046, 22034, 22099, 21906, 21941, 21803, 218		B30.3	5_2s3av40	0mw_0	0006.txt	5.62	2019-0	3-20 20:30	2000.00	3.00	400.00	2.0.6.4	B30_35_A	TCC32359_WT_1	B30_35	2019-03-20 14:	52 B	330.35
		209 206	03, 20935, 20973, 20870, 20967, 21129, 20983, 208 52, 20611, 20579, 20756, 20671, 20735, 20683, 206 26, 19912, 19887, 19646, 19924, 19922, 19841, 197		B30.3	5_2s3av40	0mw_0	0007.txt	5.68	2019-0	3-20 20:33	2000.00	3.00	405.00	2.0.6.4	B30_35_A	TCC32359_WT_1	B30_35	2019-03-20 14:	52 E	330.35
		193 183	35, 19231, 19224, 19172, 19205, 19300, 19278, 190 90, 18129, 18299, 18276, 18325, 18325, 18255, 182		B30.3	5_2s3av40	0mw_0	0008.txt	5.73	2019-0	3-20 20:36	2000.00	3.00	400.00	2.0.6.4	B30_35_A	TCC32359_WT_1	B30_35	2019-03-20 14:	52 B	330.35
		172 167 156	33, 17183, 17279, 17245, 17169, 17165, 17097, 170 89, 16673, 16693, 16633, 16598, 16507, 16457, 164 86, 15738, 15595, 15602, 15495, 15447, 15382, 155	18, 16444, 16	317, 16206, 163 524, 15511, 153	43, 16336, 16264, 1 380, 15377, 15403, 1	16239, 16011, 15355, 15346	, 16022, 16104, 1	16160, 16257, 16 15169, 15151, 15	087, 16148, 16	297, 16121, 15990, 282, 15124, 15229,	16042, 15994, 16133, 15216, 15101, 15036,	15962, 16086, 159 15067, 15142, 151	989, 15906, 159 128, 15010, 150	23, 15864, 15904, 15832, 15 91, 15117, 15059, 15011, 14	922, 15758, 15806, 1 948, 14939, 14995, 1	15814, 14979,				
		150 146 134	09, 14876, 14875, 14842, 14958, 14985, 14897, 1488 06, 14663, 14671, 14683, 14599, 14538, 14320, 144 15, 13409, 13444, 13396, 13366, 13399, 13408, 1337	1, 14876, 14 3, 14410, 14 6, 13274, 13	871, 14760, 148 428, 14509, 144 257, 13238, 130	05, 14759, 14833, 1 65, 14528, 14387, 1 187, 13140, 13130	4776, 14805, 14449, 14407, 13048, 13090	14829, 14720, 1 14320, 14319, 1 13085, 13021, 1	14790, 14746, 14 14241, 14163, 14 13081, 13055, 13	692, 14562, 14 071, 14142, 14 047, 13001, 13	533, 14594, 14658, 112, 14081, 14083, 140, 12938, 12988	14596, 14671, 14669, 14025, 13976, 13836, 13031, 13019, 12891	14764, 14677, 146 13800, 13825, 137 12903, 12887, 127	677, 14682, 146 707, 13686, 136 713, 12806, 128	16, 14606, 14567, 14590, 14 54, 13756, 13742, 13653, 13 01, 12946, 12797, 12735, 12	579, 14598, 14585, 1 655, 13608, 13552, 1 667, 12589, 12603, 1	14650, 13557, 12575				
		125	39, 12619, 12604, 12577, 12638, 12418, 12413, 123 43, 12190, 12116, 12055, 11973, 11978, 12001, 1204	i9, 12496, 12 16, 12079, 12	313, 12302, 123 047, 12034, 120	16, 12399, 12488, 1 131, 11990, 12000, 1	12367, 12323, 11944, 11840,	, 12335, 12284, 1 , 11805, 11867, 1	12327, 12335, 12 11775, 11812, 11	328, 12270, 12 837, 11900, 11	869, 12257, 12193, 95, 11875, 11838,	12207, 12200, 12169, 11785, 11824, 11737,	12259, 12228, 121 11800, 11767, 117	185, 12225, 122 781, 11852, 117	24, 12116, 12151, 12272, 12 91, 11684, 11895, 11834, 11	063, 12027, 12132, 1 788, 11716, 11680, 1	11966, 11632,				
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		759	7, 7558, 7507, 7549, 7457, 7476, 7435, 7441, 7409, 7 1, 6872, 6813, 6735, 6795, 6768, 6832, 6688, 6645, 6	431, 7455, 74 714, 6619, 66	09, 7452, 7434, 570, 6705, 6693,	7366, 7342, 7265, 7 , 6659, 6661, 6693,	7263, 7284, 72 6637, 6499, 6	225, 7261, 7180, 541, 6605, 6520,	, 7175, 7135, 716 , 6525, 6483, 654	4, 7141, 7155, 6, 6588, 6505,	153, 7108, 7170, 7 5468, 6383, 6443, 6	141, 6966, 7000, 7000, 329, 6325, 6429, 6400,	,7020,7085,7024	4, 6965, 7050, 70 5, 6302, 6346, 63	011, 6872, 6956, 6934, 6912, 396, 6392, 6299, 6305, 6319,	6882, 6913, 6830, 6 6348, 6349, 6246, 6	869, 306,				
		614 552	1, 6170, 6189, 6230, 6241, 6149, 6130, 6134, 6145, 6 1, 5585, 5554, 5523, 5557, 5454, 5455, 5447, 5446, 5	202, 6085, 61 467, 5472, 54	00, 6125, 6042, 422, 5430, 5365,	6014, 6104, 6086, 6 , 5385, 5431, 5351,	5084, 6004, 59 5263, 5286, 5	963, 5989, 5905 331, 5254, 5194	, 5870, 5909, 585 , 5252, 5172, 513	0, 5911, 5900, 5, 5172, 5182,	929, 5887, 5867, 5 5170, 5102, 5101, 5	816, 5773, 5797, 5790, 031, 5012, 5087, 5012,	, 5770, 5777, 5830 , 5031, 5088, 5053	3, 4949, 4924, 49	765, 5657, 5653, 5630, 5644, 917, 4857, 4847, 4872, 4879,	5656, 5576, 5540, 5 4785, 4845, 4804, 4	612, 1766,				
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		279	1, 2843, 2863, 2777, 2789, 2774, 2770, 2788, 2751, 2 2, 2547, 2529, 2470, 2514, 2473, 2518, 2502, 2467, 2	762, 2778, 27 486, 2517, 24	39, 2715, 2758, 430, 2518, 2413,	2755, 2740, 2745, 2 , 2423, 2446, 2424,	2766, 2726, 2 2411, 2416, 2	449, 2386, 2401	, 2678, 2744, 263 , 2422, 2356, 240	5, 2646, 2619, 19, 2376, 2433, 1	2662, 2608, 2674, 2 2370, 2357, 2336, 2	613, 2609, 2639, 2589, 305, 2316, 2289, 2295,	2602, 2609, 2635	5, 2568, 2542, 2 3, 2321, 2308, 2	542, 2551, 2546, 2502, 2493, 333, 2256, 2295, 2304, 2276,	2560, 2508, 2535, 24	253,				
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		170 152	9, 1720, 1744, 1713, 1678, 1664, 1658, 1726, 1677, 1 2, 1509, 1435, 1451, 1512, 1508, 1481, 1512, 1473, 1	703, 1690, 16 514, 1467, 15	24, 1646, 1667, 511, 1479, 1470,	1593, 1590, 1637, 1 , 1490, 1450, 1453,	1617, 1617, 16 1445, 1459, 1	607, 1628, 1597, 484, 1482, 1458,	, 1572, 1570, 158 , 1464, 1475, 145	6, 1612, 1632, <sup>1</sup> 7, 1494, 1412, <sup>1</sup>	590, 1576, 1537, 1 463, 1450, 1459, 1	554, 1524, 1607, 1590, 481, 1430, 1430, 1481,	, 1574, 1541, 1543 , 1457, 1481, 1486	3, 1580, 1532, 19 5, 1417, 1412, 14	546, 1543, 1571, 1549, 1535, 438, 1425, 1451, 1444, 1485,	1523, 1517, 1521, 1 1457, 1449, 1492, 1	521, 498,				
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		148	5, 1507, 1524, 1470, 1546, 1509, 1460, 1536, 1513, 1	499, 1540, 15	75, 1588, 1541,	1574, 1613, 1572, 1	1599, 1582, 1	553, 1625, 1626,	1649, 1638, 161	2, 1684, 1618,	692, 1651, 1663, 1	647, 1667, 1688, 1704	1662, 1714, 1717	7, 1710, 1714, 1	712, 1737, 1695, 1736, 1735,	1755, 1751, 1787, 1	787,				
		208	1, 2074, 1942, 2083, 2050, 2067, 2007, 2054, 2033, 2 5, 1000, 2026, 1064, 1092, 1088, 1020, 1021, 1054, 1054, 1055, 1050, 1051	038, 2087, 20	146, 2095, 2069,	2088, 2068, 2047, 2088, 1908, 1908, 1908, 2068, 2047, 2019	2021, 2058, 2	046, 2066, 2059,	, 2101, 2106, 205	4, 2051, 2060, 2	2064, 2014, 2037, 2	033, 2029, 2013, 2034, 522	, 2071, 2048, 2066	5, 1994, 2014, 20	064, 2021, 1995, 2018, 2017,	2013, 2041, 2033, 20	035,				
		13,	6, 12, 9, 11, 12, 12, 7, 11, 14, 11, 12, 16, 14, 7, 22, 20, 1	6, 20, 21, 16,	26, 46, 30, 40, 4	14, 38, 45, 42, 43, 55	i, 66, 51, 49, 6	7, 63, 74, 85, 110	), 102, 113, 107, 1	125, 143, 130, 1	79, 199, 262, 351, 6	63, 1289, 2659, 5235, 9	9051, 14252, 1976	55, 24927, 2875	5, 30918, 32254, 33042, 330	46, 33207, 33238, 33	3221,				

Rama

Trans MAN

	HPLC data and transformed Raman data are copied into	
Raman_HPLC_Join © B500mL_003_C	Datasets within a LabKey Study.	Pacific
Report Source Help		NATIONAL LABORATORY
⊟ Attachment output	An R report is used to join the Datasets on timestamp and to	
Text output file (click to download)	generate a file for training a chemometric model.	

### Joining Raman and HPLC -> Pirouette

#### User Guide

This R report generates a file to be used to build a pirouette model that predicts concentrations of compo same time to create training data.

#### **Required Libraries**

- Rlabkey
- data.table
- glue

#### **Adjustable Parameters**

The adjustable paramenters are documented throughout the report, but the most essential are directly be

- raman\_table corresponds to the name of the dataset containing the raman in this study
- hplc\_table likewise corresponds to the name of the dataset containing the HPLC in this study
- subject\_id corresponds to the SubjectID you want to generate a file from.
- training\_names are the Field Names of the HPLC columns that you want to train the model on. This
- table set TRUE if you want to see a table displayed of the join before downloading. Set FALSE to h

```
raman_table = 'Raman_Transformation'
hplc_table = 'HPLC_Sugars_OrgAcids_BPD'
subject_id = 'Y-7208_B500mL_003'
training_names = c('Glucose_g_L', 'Xylose_g_L', 'Citric_Acid_g_L', 'Xylitol_
table = FALSE
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## Chemometric data input file showing one of the Raman spectra it contains

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341 316	25, 34 99, 31	167,	34057, 31390,	33990, 31328,	33924, 31238,	33760, 38958,	33542 30783	33556	, 33399, , 30337,	33521, 30097.	33238, 29899.	33186, 29786.	33197 29483	33000	, 3310	2, 3296 1, 2915	3, 329 2, 290	0, 32659 3, 28740	, 32758	, 32714, 28446,	32431, 28458,	32360, 28444,	32158, 28269.	32028, 28138.	31959, 28244,	31868, 28107.	31853, 281566, 2815666, 2815666, 2815666, 2815666, 2815666, 2815666, 2815666666666666666666666666666666666666	31745, 316 27932, 278	674, 851,
276	74, 27 23, 25	519,	27383, 26158	27215, 26072.	26934, 26141.	26930, 26262.	27013	26933	, 26814,	26742, 26136.	26771, 26399.	26843, 26468.	26583 26462	26673	2668	0, 2639 0, 2701	1, 2654	9, 26515	26331	26383, 27155.	26386, 26845.	26541, 26774.	26405, 26834.	26460, 26983.	26389, 26999.	26261, 27314.	26270, 27518.	26844, 268	973, 542.
273	88, 27 68, 27	266,	27864,	27238, 27675.	27239, 27688.	27246, 27738.	27500	27754	27966	28018, 27456.	28013, 27283.	28201, 27408.	28489	28763	2949	0, 3041 2, 2751	2, 308	5, 30628	29830	29395, 27565.	28836, 27634.	28735, 27776.	28526, 27889.	28208, 27861.	28253, 27767.	27867, 28845.	27928, 28078.	27868, 278	859, 294.
283	31, 28	146,	28528	28402, 28246	28344, 27981.	28238, 27832.	28146	28180	28425	28476, 27487.	28558, 27364	28585, 27249.	28688	28737	2874	1, 2869	7, 284	7, 28313	28841	27983, 27156	28246,	28832, 26963.	28109, 27829.	28180, 27814.	28185,	28070, 26833.	28070, 26962	27987, 278	822,
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113	88, 11 91, 10	386, 388,	11377, 10744,	11421, 10696,	11338, 10701,	11412, 10619,	11277	11269	, 11230, , 10547,	11219, 10561,	11182, 10496,	11200, 10475,	11123	, 11162	, 1118	1, 1113 4, 1030	1, 111 6, 104	5, 11084 1, 10300	, 11018 , 10382	, 11027, , 10394,	10940, 10254,	11005, 10292,	10279,	10925, 10198,	10926, 10143,	10920, 10117,	10878, 10093,	10885, 107 10162, 100	793, 071,
100	48, 10 3, 939	932, 9, 94	10021, 01, 94	10084,	10024, 4, 9347	10012, 9267,	9952, 9317,	9930, 9341,	9916, 97 9380, 93	84, 998 56, 928	5, 9811 4, 9225	, 9685, , 9284,	9707, 9122,	9742, 9202,	9738, 9113,	9758, 9 9898, 9	753, 9 084, 9	13, 9564 14, 9067	, 9593, , 9038,	9621, 9 8990, 8	526, 94 977, 89	92, 950 94, 901	5, 9607 7, 8893	9503, 8842,	9650, 8969,	9536, 9 8923, 8	514, 956 881, 890	7, 9490, 7, 8891,	
896 825	7, 884 2, 813	5, 88 9, 82	12, 80 13, 81	73, 885	4, 8854 8, 8229	, 8773, , 8169,	8862, 8106,	8839, 8132,	8785, 87 8013, 81	44, 873 59, 814	2, 8694 2, 8060	, 8679, , 8081,	8786, 7947,	8589, 7979,	8614, 8007,	8587, 8 7989, 7	590, 8 918, 7	43, 8520	, 8582, , 7946,	8684, 8 7851, 7	413, 84 849, 78	15, 840 30, 782	5, 8407 2, 7814	, 8480, , 7775,	8298, 7671,	8372, 8 7685, 7	334, 824 609, 763	5, 8231, 3, 7639,	
766	3, 774 2, 681	9, 76 3, 67	32, 70 54, 68	63, 764 30, 675	2, 7551 7, 6768	, 7475, , 6723,	7430, 6746,	7399, 6697,	7413, 72	99, 733 69, 656	7, 7409 5, 6602	, 7377, , 6660,	7315, 6597,	7268, 6625,	7362, 6623,	7309, 7 6594, 6	158, 7: 597, 64	31, 7145 72, 6473	, 7141, , 6528,	7065, 7	101, 70 413, 63	44, 699 57, 637	5, 7013, 3, 6327,	, 6991, , 6349,	6925, 6321,	6938, 6 6298, 6	858, 690 270, 627	5, 6874, 2, 6282,	
628 585	8, 618 8, 574	8, 62 8, 58	48, 62 30, 58	32, 625 25, 575	2, 6161 2, 5777	, 6170, , 5712,	6167, 5777,	6859, 5634,	6201, 61 5752, 50	68, 613 73, 572	7, 6897 2, 5666	, 6112, , 5615,	6105, 5610,	6007, 5683,	6085, 5570,	6859, 6 5640, 5	001, 60 577, 55	31, 6065 93, 5548	, 6007, , 5599,	5910, 6 5561, 5	084, 59 494, 54	80, 5871 70, 555	3, 5857, 5, 5452,	, 5850, , 5537,	5912, 5409,	5927, 5 5384, 5	749, 584 365, 534	4, 5844, 9, 5307,	
541 488	2, 540 8, 490	9, 52 7, 49	52, 53 16, 48	156, 528 146, 483	2, 5279 3, 4913	, 5283, , 4897,	5314, 4839,	5254, 4782,	5261, 52 4798, 47	26, 514 81, 473	1, 5132 5, 4688	, 5193, , 4710,	5209, 4708,	5191, 4762,	5096, 4767,	5137, 5 4665, 4	158, 5: 692, 44	30, 5101 02, 4601	, 5091, , 4673,	5033, 4 4687, 4	961, 50 601, 46	79, 503 14, 454	1, 5074, 7, 4651,	, 5075, , 4478,	5008, 4460,	4927, 4 4534, 4	969, 495 474, 451	4, 4967, 3, 4471,	
445	2, 447 1, 410	2, 44 1, 40	83, 43 31, 39	91, 436 67, 405	3, 4375 5, 3982	, 4434, , 4041,	4411, 4001,	4408, 3949,	4446, 43 4855, 39	90, 432 72, 395	5, 4339 2, 3996	, 4287, , 3949,	4276, 3973,	4306, 3960,	4232, 3947,	4163, 4 3850, 3	191, 43 895, 34	159, 4184 188, 3900	, 4252, , 3832,	4201, 4 3867, 3	196, 41 866, 38	69, 417 68, 382	7, 4157, 3, 3901,	, 4203, , 3748,	4113, 3856,	4129, 4 3805, 3	173, 413 811, 379	8, 4141, 8, 3798,	
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317 287	5, 312 4, 290	1, 31 5, 28	43, 31 85, 28	14, 308 92, 291	4, 3105 1, 2839	, 3113, , 2897,	3144, 2917,	3107, 2821,	3081, 30 2825, 28	43, 301 19, 284	7, 3056 8, 2855	, 2986, , 2829,	2982, 2764,	3039, 2809,	3003, 2778,	2967, 3 2762, 2	825, 29 818, 21	187, 3035 174, 2743	, 3026, , 2757,	2937, 2 2764, 2	925, 29 695, 27	51, 296 50, 271	7, 2929, 4, 2695,	, 2973, , 2758,	2955, 2706,	2926, 2 2713, 2	928, 292 754, 274	8, 2895, 5, 2593,	
271 242	1, 273 6, 241	5, 26 4, 24	94, 21 29, 21	06, 269 90, 241	4, 2678 3, 2355	, 2615, , 2374,	2605, 2388,	2610, 2342,	2577, 26 2390, 23	63, 257 53, 237	5, 2636 1, 2363	, 2609, , 2384,	2616, 2334,	2605, 2380,	2629, 2273,	2544, 2 2362, 2	507, 2 267, 2	39, 2521 96, 2264	, 2523, , 2246,	2513, 2 2189, 2	485, 24 272, 22	28, 248	2, 2470, 5, 2265,	2488, 2252,	2482, 2278,	2511, 2 2292, 2	462, 242	9, 2446, 8, 2236,	
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233 223	6, 231 0, 223	4, 23 7, 22	23, 23 29, 23	98, 233	3, 2346 9, 2110	, 2309, 2104,	2323, 2082,	2341, 2100,	2370, 24 2115, 21	04, 230 01, 211	5, 2392 7, 2079	, 2387, 2064,	2346, 2125,	2372, 2850,	2316, 2033,	2339, 2 2119, 2	431, 23 886, 24	33, 2356 53, 2083	, 2325, 2846,	2393, 2 2034, 2	362, 23	48, 227	5, 2339, 7, 2031,	2315, 2075,	2248, 2071,	2250, 2 2014, 1	223, 224 989, 201	2, 2210, 0, 2015,	
194 181	8, 201 4, 177	5, 20 5, 17	13, 19 74, 17	89, 193 42, 175	6, 1957 9, 1771	, 1955, 1792,	1986, 1767,	1898, 1751,	1867, 19	12, 189	9, 1867 5, 1699	, 1821, 1729,	1871, 1701,	1818, 1676,	1843, 1701,	1884, 1 1661, 1	823, 14 685, 10	28, 1825	1777, 1788,	1817, 1 1718, 1	789, 17	51, 175	1, 1823 1, 1657	1768, 1654,	1884, 1659,	1884, 1 1625, 1	789, 179	9, 1774, 7, 1649,	
162 172	1, 159 4, 169	2, 16 0, 17	92, 10 15, 17	49, 162	5, 1635 7, 1712	, 1639, , 1696,	1617, 1733,	1649, 1783,	1686, 16 1760, 17	69, 170 52, 172	0, 1630 1, 1780	, 1632, , 1785,	1687, 1766,	1648, 1811,	1694, 1742,	1685, 1 1733, 1	653, 10 760, 13	22, 1643	, 1707, , 1815,	1710, 1 1779, 1	676, 16 811, 17	28, 171	7, 1691, 3, 1783,	, 1709, , 1784,	1673, 1840,	1722, 1 1827, 1	675, 168 829, 186	1, 1727, 8, 1866,	
186	4, 183 2, 204	5, 18 8, 20	38, 18 11, 19	79, 185	5, 1909 6, 2058	, 1861, 2033,	1922, 2878,	1874, 2828,	1909, 18 2847, 26	94, 192	3, 1938 7, 2059	, 1929, 2884,	1978, 2142,	1944, 2897,	1915, 2153,	1963, 1 2139, 2	997, 19 899, 21	77, 1923	1940, 2095,	1983, 1 2118, 2	939, 19	68, 199 59, 212	7, 2010	2014, 2195.	1975, 2178,	1953, 1 2147, 2	963, 199 166, 214	4, 2000, 7, 2138,	
216 218	4, 216 8, 222	1, 21 2, 22	09, 21 05, 21	75, 218	7, 2192	, 2193, 2231,	2181, 2188,	2179, 2230,	2191, 21 2229, 22	80, 219	8, 2182 2, 2238	, 2210, 2250,	2174, 2201,	2216, 2157,	2236, 2218,	2194, 2 2193, 2	218, 2	86, 2207 92, 2179	, 2222, 2203,	2284, 2 2174, 2	261, 22	66, 220	7, 2226	2189, 2158,	2246, 2182,	2201, 2 2126, 2	185, 221	4, 2239, 4, 2143,	
216	8, 218 539126	7, 20 53059	95, 21 744, 6	10, 207	4, 2084 4485308	, 2075, 93	2016,	2031,	2056, 20	10, 205	1, 1996	, 1989,	1958,	1958,	1919,	1936, 1	895, 14	80, 1899	, 1852,	1770, 1	760, 16	96, 167	5, 1541	, 25.83	9973781	8727, 1	4.444176	5551736,	
#S,	2.498	_B500	.mL, 1	8, 10, 1	12, 8,	13, 15,	13, 14	1, 13,	20, 9, 1	3, 22,	15, 19,	26, 24	, 25, 3	35, 36,	47, 3	ə, sə,	38, 45,	42, 47,	55, 57	, 59, 57	, 81, 6	a, 68, 9	92, 89,	82, 10	0, 114,	115, 1	16, 109,	153, 175,	

The R output file containing Raman spectra joined with HPLC data on timestamp is loaded into Pirouette chemometric software from Infometrix (Bothell, WA).

![](_page_18_Picture_1.jpeg)

Partial Lest Squares (PLS) multiple regression models are then created to predict concentrations of culture broth components in real time during bioreactor operations.

![](_page_18_Figure_3.jpeg)

![](_page_19_Picture_0.jpeg)

The Raman PLS model is integrated with a PID algorithm for fed-batch control of a hydrolysate feed pump.

In our initial test, the system automatically fed hydrolysate to the bioreactor to maintain glucose levels between 0.5 and 3 g/L for 72 hours (green line in chart).

![](_page_19_Figure_3.jpeg)

## Vision for expanding chemometric data integration within LabKey

![](_page_20_Figure_1.jpeg)

![](_page_21_Picture_0.jpeg)

# Ultimate Goal: Spectroscopy integration within a chemostat control system for directed evolution

![](_page_21_Figure_2.jpeg)

A Sixfors multi-vessel bioreactor array is being retrofitted with an HC900 programmable logic controller to create a "fitness landscape explorer" for automatically improving growth rate and productivity of industrial microbes across multiple ranges of culture conditions and feedstock compositions.

Examples of technical support that we have received from LabKey

-	Title 🛇	Priority 🗢	Status 🗢	Target Release 🤇
	Files Web Part Error - loss of access to files within a folder	2	open	
	LDAPS?	3	closed	
	out of memory crash	3	resolved	
	Tranformation script for OOR indicator	3	closed	
	Out of Range Indicator	3	open	
	server state management - recovery	3	closed	
	Better understanding of docker integration	3	closed	
	Configuring scripting engines	3	closed	
	Recommendations on "safe" R packages?	3	closed	
	Schedule Training (Admin, User and Developer)	3	open	
	MatLab integration with LabKey	3	resolved	19.3 (Nov)
	Jupyter Integration with LabKey	3	closed	
	Set up RStudio Integration	3	closed	
	LK support for timestamp and window SQL commands and functions	3	resolved	
	General Assay -Expected rate of writing to database?	3	open	18.1 (Mar)
	LIRL specification behaves differently after study export and import	3	onen	
	Problems with folder import/export issues across LabKey servers	3	resolved	
		3	anan	
	R Package Riabkey fails to complie on RHEL linux	2	open	
	Workaround for mandatory use of calendar date or visit ID with participant ID in studies	2	resolved	19.3 (Nov)
	Amount of idle time before user logoff	4	resolved	19.1 (Mar)
	Can you confirm mitigation in SAML 2018 impersonation vulnerabilities?	4	resolved	

![](_page_22_Picture_2.jpeg)

Copy-To-Study now provides option to show time as well as date – important for time series data (Thanks, LabKey!)

![](_page_23_Picture_1.jpeg)

Assay List / HPLC\_Sugars\_OrgAcids\_BPD

### Copy to Raman\_Transform\_Study Study: Verify Results DAutomation\_Dev

Participant IDs and Dates are required for all rows.

	Copy to Stu	dy Re-Valid	ate Display Date lime	Cancel										
	Specimen Match	Originating Run	Participant ID	Date	Timepoint Preview	Sample ID	Culture Age	Strain Line ID	Experiment	Glucose (g/L)	Xylose (g/L)	Citric Acid (g/L)	Xylitol (g/L)	F (
	<b>x</b> ?	VIEW RUN »	Y-7208_B500mL_003	2019-09-06 16:49	Day 29	B500mL_003_ACF_002	1.76	Y- 7208_B500mL_003	B500mL_003	27.54	15.59	0.06	0.43	
	<b>x</b> ?	VIEW RUN »	Y-7208_B500mL_003	2019-09-06 18:19	Day 29	B500mL_003_ACF_004	3.26	Y- 7208_B500mL_003	B500mL_003	26.83	14.96	0.05	0.42	
	<b>x</b> ?	VIEW RUN »	Y-7208_B500mL_003	2019-09-06 19:49	Day 29	B500mL_003_ACF_006	4.76	Y- 7208_B500mL_003	B500mL_003	26.56	14.88	0.06	0.37	
	<b>x</b> ?	VIEW RUN »	Y-7208_B500mL_003	2019-09-06 21:19	Day 29	B500mL_003_ACF_008	6.26	Y- 7208_B500mL_003	B500mL_003	26.33	14.96	0.06	0.38	
)	<b>x</b> ?	VIEW RUN »	Y-7208_B500mL_003	2019-09-06 22:49	Day 29	B500mL_003_ACF_010	7.76	Y- 7208_B500mL_003	B500mL_003	26.75	15.46	0.07	0.42	
)	<b>X</b> ?	VIEW RUN )	Y-7208_B500mL_003	2019-09-07 00:19	Day 30	B500mL_003_ACF_012	9.26	Y- 7208_B500mL_003	B500mL_003	24.86	14.86	0.06	0.44	
)	<b>X</b> ?	VIEW RUN »	Y-7208_B500mL_003	2019-09-07 01:49	Day 30	B500mL_003_ACF_014	10.76	Y- 7208_B500mL_003	B500mL_003	24.26	15.35	0.08	0.40	
	<b>X</b> ?	VIEW RUN )	Y-7208_B500mL_003	2019-09-07 03:19	Day 30	B500mL_003_ACF_016	12.26	Y- 7208_B500mL_003	B500mL_003	22.09	15.30	0.05	0.46	

## Acknowledgements

![](_page_24_Picture_1.jpeg)

ENERGY Energy Efficiency & BIOENERGY TECHNOLOGIES OFFICE

BETO Technology Manager: Beau Hoffman

![](_page_24_Picture_4.jpeg)

**FCIC Task 4 Data Integration:** Rachel Emerson (INL), Shaun O'Leary (PNNL), Bruce Wilson (ORNL), Robert Kinoshita (INL), Alan Chappell (PNNL), Lorenzo Vega-Montoto (INL), David Sievers (NREL), Stan Martin (ORNL), Matt MacDuff (PNNL), Oslo Jacobsen (LBNL)

![](_page_24_Picture_6.jpeg)

**PNNL Bioprocess Development:** Isaiah Lemmon, Todd Hart, Beth Hofstad, Kyle Pomraning, Marie Swita

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